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Methyl 3-benzoyl-3-(6-methyl-2-pyridyl)-2-phenylacrylate

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Key indicators

Single-crystal X-ray study
T = 213 K
Mean σ(C–C) = 0.005 Å
R factor = 0.062
wR factor = 0.148
Data-to-parameter ratio = 13.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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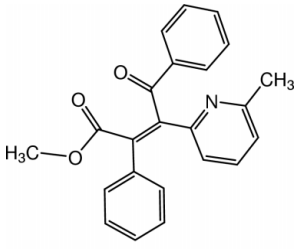
The benzoyl and phenyl rings of the title molecule, $C_{23}H_{19}NO_3$, are oriented at angles of 79.9 (1) and 70.8 (1)°, respectively, with respect to the pyridine ring. The weak C—H···O intermolecular hydrogen bonds link the molecules to form infinite one-dimensional chains along the *a*-axis direction.

Comment

Photo-induced oxygenation reactions of indolizine derivatives have been intensively investigated (Tian *et al.*, 2001). In a continuation of this work, we report here the crystal structure of the title compound, (I), which was isolated from the reaction mixtures of the photoinduced oxygenation reaction mixture of 5-methyl-2-phenylindolizine.



(I)

The observed bond lengths in (I) (Fig. 1) lie within the normal ranges (Allen *et al.*, 1987) and bond angles show normal values. Atoms C7, C8, C9, C14, C15 and C21, linking the three aromatic rings and the methyl ester group, are coplanar. This plane make dihedral angles of 17.5 (1), 78.0 (1) and 71.3 (1)°, respectively, with the pyridine, benzoyl and phenyl rings, and the methyl ester group is twisted away by 46.0 (1)°. The benzoyl and phenyl rings are oriented at angles of 79.9 (1) and 70.8 (1)°, respectively, to the pyridine ring. In the crystal, weak C—H···O intermolecular hydrogen bonds link the molecules, translated along the *a*-axis direction to form infinite one-dimensional chains (Table 1).

Experimental

The title compound was prepared by photo-induced oxygenation reaction of 5-methyl-2-phenylindolizine in a methanol-containing benzene solution and was isolated from the reaction mixture by column chromatography on silica gel. Single crystals were grown by slow evaporation from a petroleum ether (333–363 K)–ethyl acetate (8/1, *v*/*v*) solvent system.

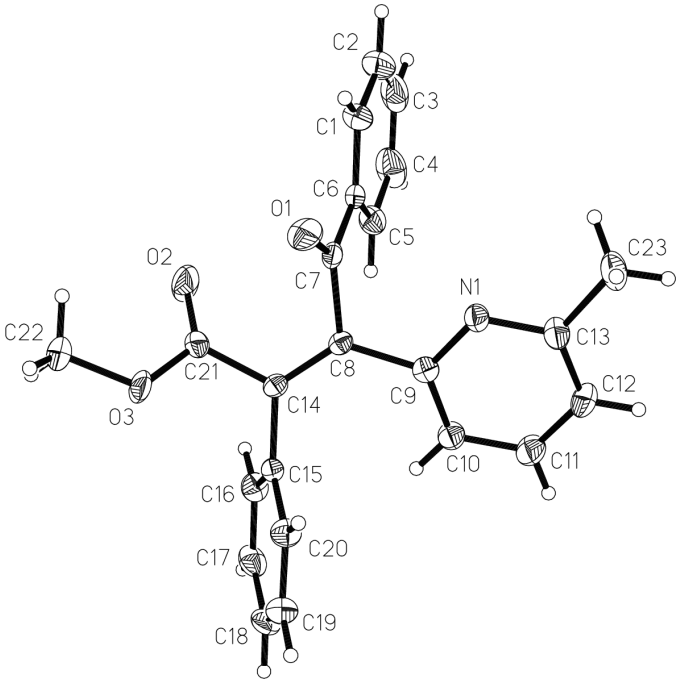


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Crystal data

$C_{23}H_{19}NO_3$	D_x = 1.276 Mg m^{-3}
M_r = 357.39	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3918 reflections
a = 8.6711 (3) Å	θ = 2.7–28.3°
b = 23.2413 (7) Å	μ = 0.09 mm^{-1}
c = 10.0129 (3) Å	T = 213 (2) K
β = 112.744 (1)°	Needle, colorless
V = 1861.0 (1) Å^3	0.38 × 0.14 × 0.12 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	1711 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.119
Absorption correction: none	θ_{max} = 25.0°
8684 measured reflections	$h = -10 \rightarrow 10$
3233 independent reflections	$k = -26 \rightarrow 27$
	$l = -7 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.062	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.148	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
S = 0.84	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
3233 reflections	Extinction correction: *SHELXTL*
247 parameters	Extinction coefficient: 0.024 (2)
H-atom parameters constrained	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O1^{i}	0.93	2.56	3.170 (5)	124

Symmetry code: (i) $x-1, y, z$.

The H atoms were fixed geometrically and treated as riding atoms on the parent C atoms, with aromatic C—H = 0.93 Å and methyl C—H = 0.96 Å, and with displacement parameters $U_{iso}(H) = 1.2U_{eq}(C)$. Owing to a large fraction of weak data at higher angles, the 2θ maximum was limited to 50°. The large value of R_{int} is a result of the poor quality of the crystal.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* and *SADABS* (Sheldrick, 1996); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

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